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RICHMOND, VIRGINIA

To: • Dr. E. B. Sanders,
From: • Y. Houminer
Subject: • Plans and Objectives of Project 2515 for 1982

Date: October 27, 1981

FLAVOR-RELEASE CHEMISTRY

Work during 1982 will focus on both synthetic and pyrolytic aspects of different flavor release systems.

GENERAL OBJECTIVES

1. To develop release systems for flavors which cannot be added directly to tobacco because of either their high volatility or their very low odor threshold. To obtain patent position in this area.
2. To examine the relationships between structure and release efficiency in a variety of systems. To carry out systematic research in that direction so that structure-efficiency correlation can be obtained and used in the future for the design of flavor release compounds.
3. To use different release systems as models for understanding the mechanism of smoke formation. In particular we would like to understand the factors affecting sidestream and mainstream deliveries.
4. To provide assistance to development upon request, in connection with objective No. 1.
5. To carry out research in the area of cooked flavors, focusing mainly on the melanoidin fraction of the cooked flavor composition. To isolate, characterize and identify the components of this fraction and to study their pyrolytic behavior.
6. To continue carrying out basic research related to some new and important scientific discoveries made during our routine research in connection with the above objectives.

PLANS

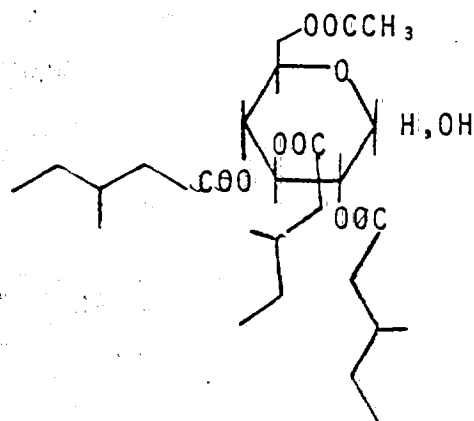
1. Sugar-based release systems (acid release).

Last year we had spent much of our time on the purification and structure determination of sucrose-tetraesters isolated from Oriental tobacco. Unfortunately, during the recent 1981 TCRC

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meeting researchers from the USDA reported the isolation of the same product. We are now waiting to receive more detail from the USDA people about their work. Nevertheless, we will make an effort to synthesize at least one of the sucrose tetraesters. We will first develop synthetic routes to D-glucose tetraester I and then study the feasibility of coupling it with a suitably protected D-fructose. We will also explore the possibility of preparing other disaccharides derived from I.



We will continue our synthetic efforts in preparing positional isomers of glucose mono esters. We will also try to increase the number of esters per glucose unit. This series of compounds will be pyrolyzed and is also targeted to meet goals given in objectives 1 and 2. We also plan to explore the use of partially acylated starch as an acid release agent. (Continuing 4th Quarter).

2. Sugar-based release systems (phenol release).

Our initial work in the area of disaccharide glycosides appears to be very promising. We will optimize synthetic procedures and extend them to a variety of phenolic flavorants. We will carry out smoke studies to demonstrate the advantage of disaccharides as carriers. These systems may turn out to be useful for MS/SS delivery ratio studies. (3rd Quarter).

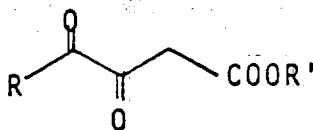
3. Sugar-based release systems (thiol release).

In the past we have looked at ethylthioglucooside as a potential release precursor for ethanethiol. We plan to further explore this area by preparing a number of thioglycosides of disaccharides and study their pyrolytic behavior (3rd Quarter).

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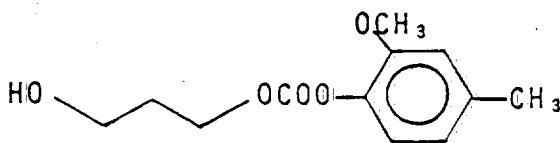
4. Ketone and diketone release.

We have nearly completed our work in the area of β -ketoesters derived from sugars. The material will be summarized and submitted as a patent disclosure (1st Quarter). We plan to extend this research to 1,2-diketones, such as biacetyl, by preparing release systems having the general structure II, where R' is a suitable carrier such as glucose, glycerol etc. (2nd Quarter)

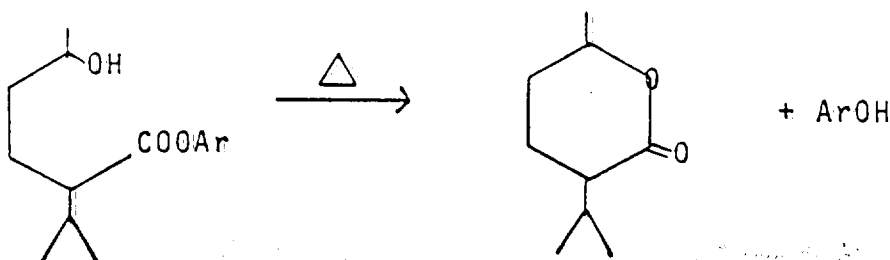


5. Phenol-release from low molecular weight precursors.

We have recently concluded that glycerol does not serve as a good carrier for the release of phenols from its carbonates. However, the monocarbonate derived from 1,3-propanediol (III) appears to be a more promising release agent. We will prepare a few analogues of III and study their pyrolysis. We also plan to use 5-hydroxyesters, such as IV, for the release



of phenols. In the following example the resulting lactone is a tobacco identical compound (3rd Quarter).



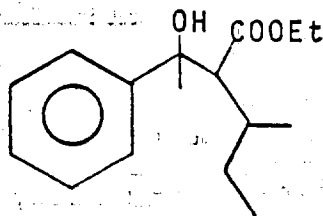
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6. Glycerol-based acid release systems.

We have started to explore this area during the past year and plan to continue in the same direction. In particular we will evaluate the mono-esters that have already been prepared. We plan also to test glyceraldehyde as a carrier for acids. We expect to observe differences for glyceraldehyde esters as compared to glycerol esters. (1st Quarter).

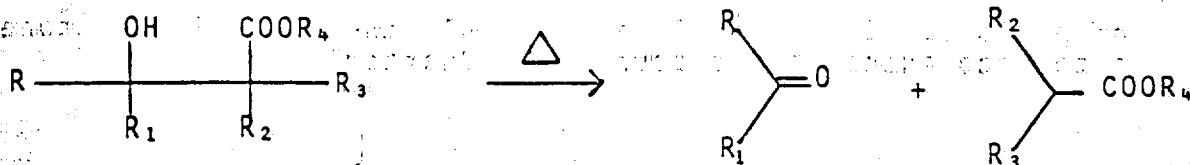
7. Ketone and ester release from β -hydroxyesters.

During the past year we have prepared a very good release system for ethyl 3-methylvalerate. This system (V) which is a β -hydroxyester, is now being tested by Flavor Development. We plan to supply Development with a large quantity of V upon request.



V

We plan to further explore the pyrolytic behavior of a large number of β -hydroxyesters (VI) where we hope to be able to establish a correlation between structure and release efficiency. We will focus on steric and electronic effects both on the α - and β -positions of the propionate skeleton. This research may also help us in meeting some of the goals stated in



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general objectives 2 and 3. We will also explore the use of these systems for the release of ketones by condensing them with high molecular weight esters that have no significant flavor properties (continuing 4th Quarter).

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8. Cooked flavors.

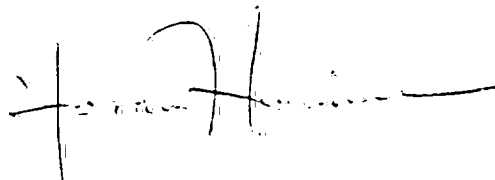
We have recently started to work in this area. We plan to develop methods that will enable us to isolate the melanoidin fraction from the cooked flavor mixture. We will try to characterize these compounds and in particular focus on their pyrolytic behavior (2nd Quarter).

9. Polymeric release agents.

In the past few years a large number of polymeric release systems have been prepared. During the coming year we plan to evaluate some of these polymeric precursors. (2nd Quarter).

10. Basic research - N.M.R. studies.

We plan to continue our study in the area of long range coupling through 4σ -bonds. To the best of our knowledge we are the first to observe such a coupling between a CH_3 and OH group in a none rigid system. We plan to publish these results next year (1st Quarter).



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